

DNS of premixed flames

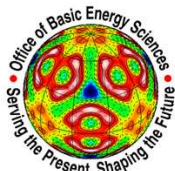
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Supported by
Division of Chemical Sciences, Geosciences, and Biosciences,
Office of Basic Energy Sciences, DOE
SciDAC

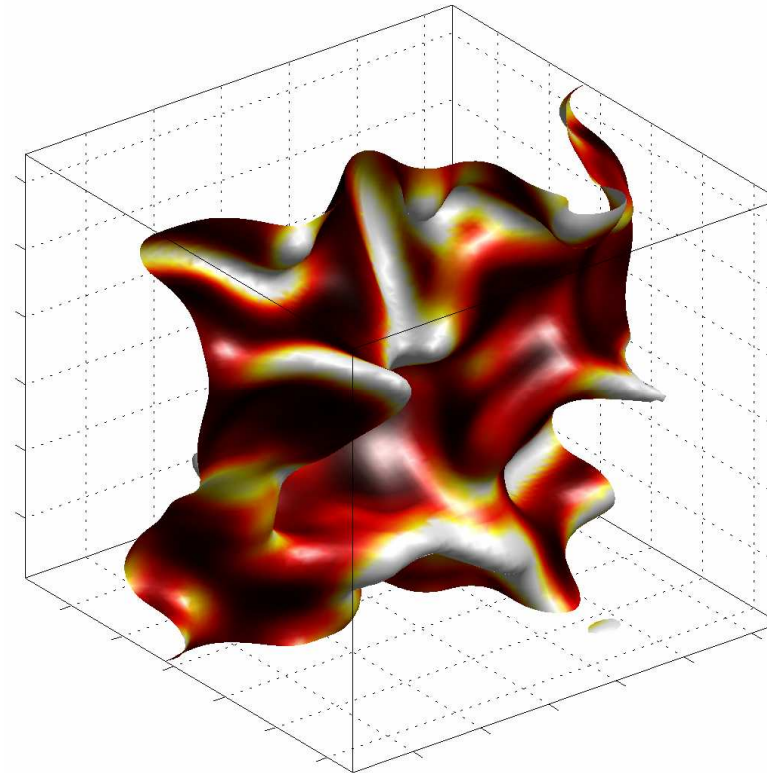
Computing: LBNL NERSC, ORNL NLCF



DNS - Past Simulations



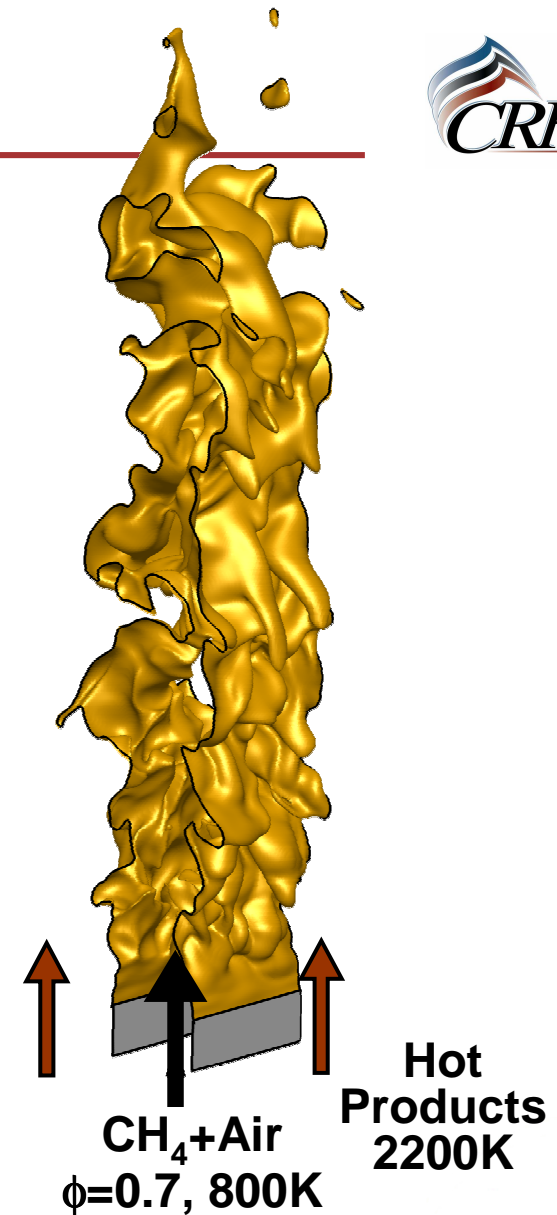
- Flame interacts with decaying turbulence in a box.
- Not stationary.
- No mean shear.
- Often, either 2D with detailed chemistry or 3D with simple chemistry.
- Limited opportunities for model validation.



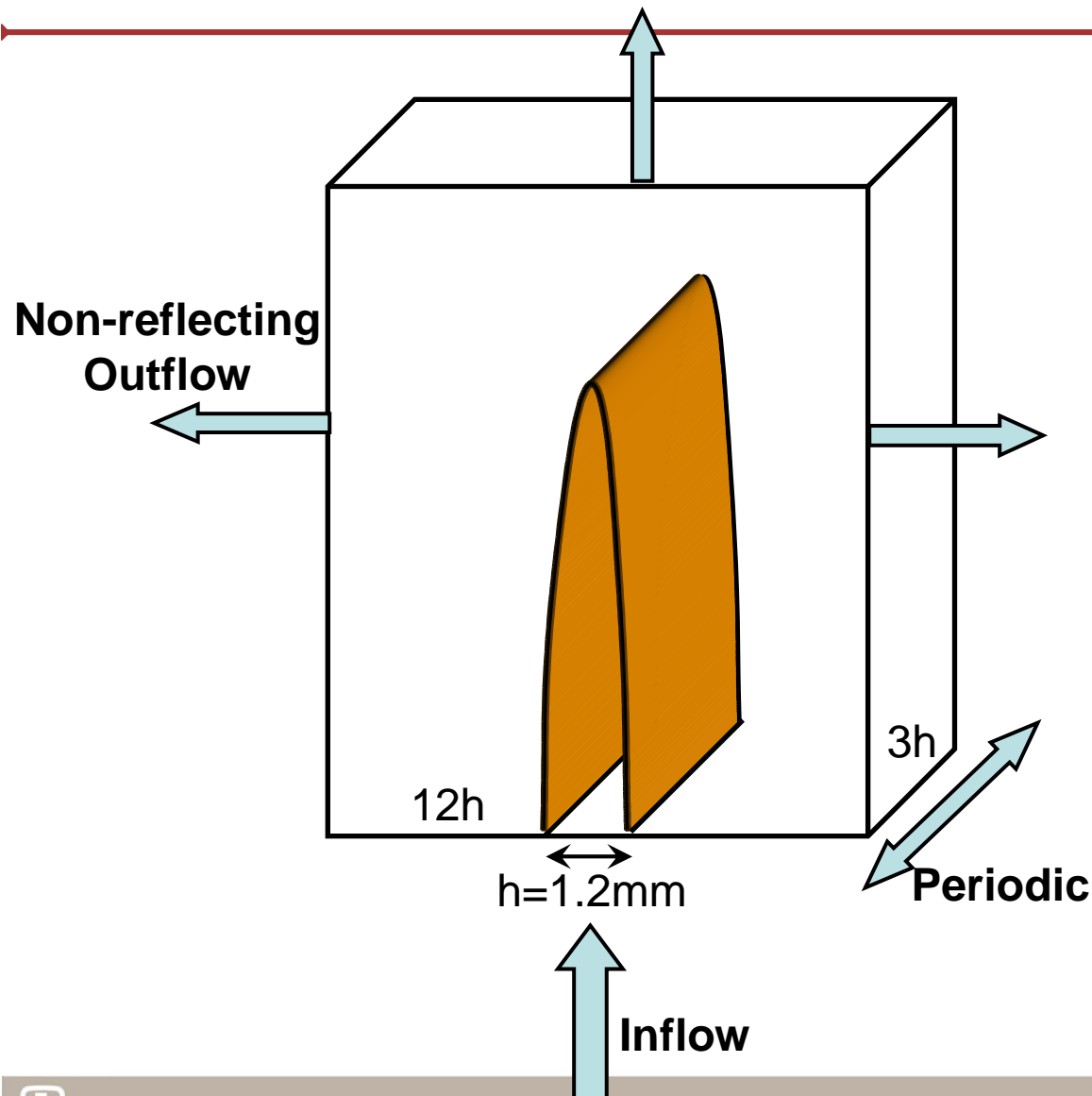
Present Simulation



- 3D slot burner turbulent Bunsen flame
 - Spatially developing and stationary configuration
- CH_4 -Air mixture ($\phi=0.7$) flow through a central jet
- Reactants surrounded by hot product coflow
 - Similar to pilot flame in experiments
- Turbulent flow with mean shear



Simulation Details

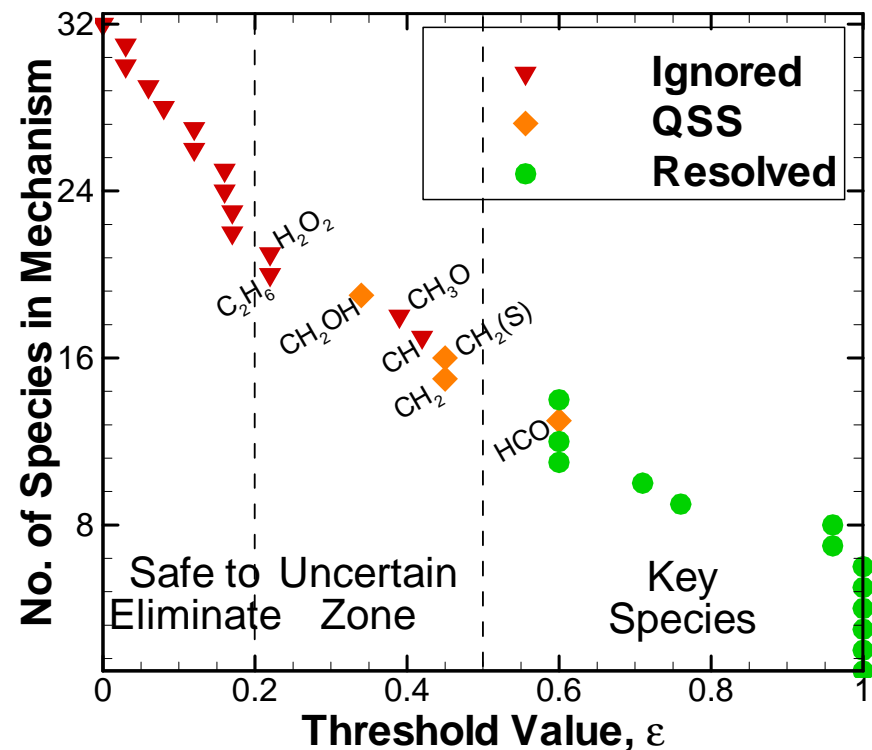


- Compressible reacting Navier-Stokes equations.
- High fidelity numerical methods.
 - 8th order finite-difference
 - 4th order explicit RK integrator
- Structured cartesian mesh
- Stretched in cross-stream direction
- Uniform in stream-wise and span-wise direction
- $20\mu\text{m}$ resolution
- Constant Lewis numbers
- Chemistry: 13 species reduced mechanism
(thanks to T. Lu, C.K. Law)

Chemistry Model



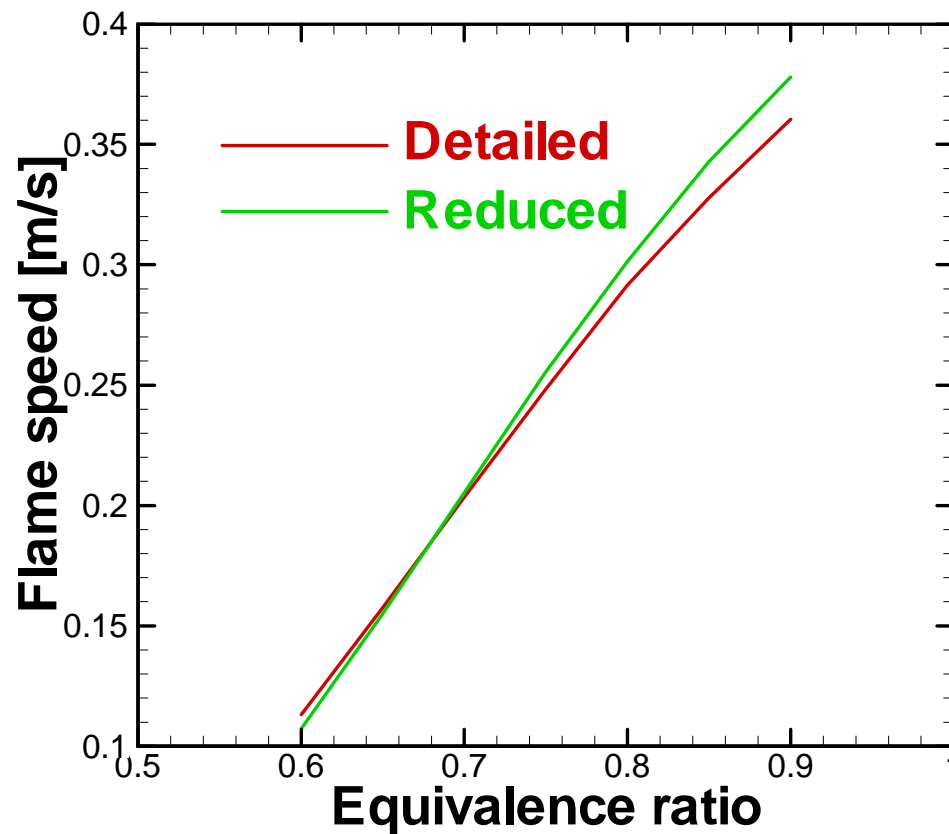
- Reduced mechanism has been derived specifically for lean premixed flame DNS.
- Starting mechanism is GRI-1.2
- Systematic reduction by analyzing representative reaction states
 - Directed relation graph (DRG)
 - Sensitivity analysis
- New reduced mechanism
 - 73 elementary reactions
 - 13 resolved species
 - 4 quasi-steady state species
 - Algebraic relations
 - No costly iterations
 - No convergence issues



Mechanism Validation



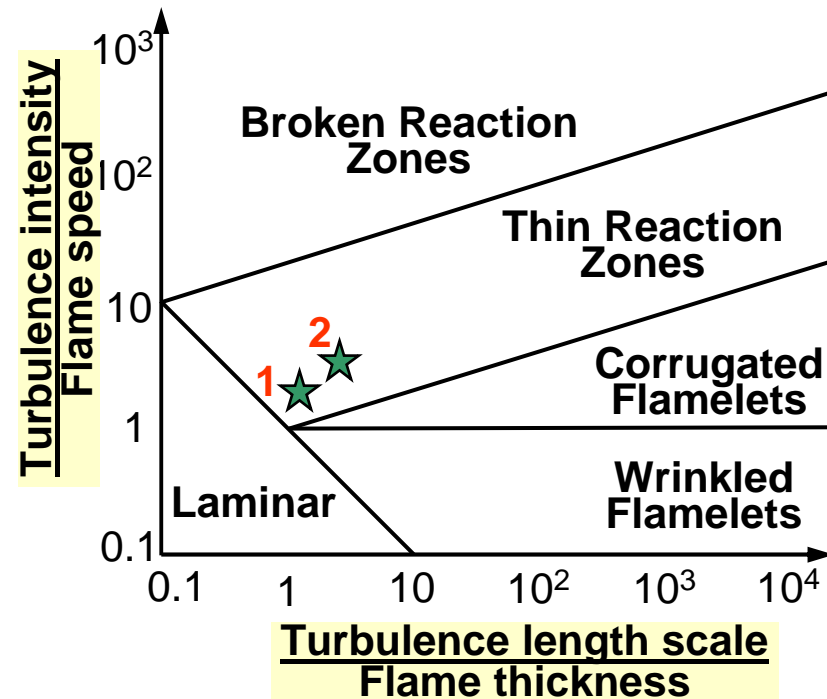
- Good agreement obtained for flame speed and structure at lean conditions.



Combustion Regimes



- Flamelets regime
 - Eddies cannot penetrate the flame
 - Flame structure is intact
- Thin reaction zones (TRZ) regime
 - Eddies can penetrate the flame structure
 - Preheat zone alone is affected
 - Reaction zone is intact
 - Modeling is a challenge
- Lean premixed combustion
 - Flame is slower and thicker
 - More likely to be in TRZ regime



'Turbulent Combustion'
by Peters(2000)

Simulation Parameters

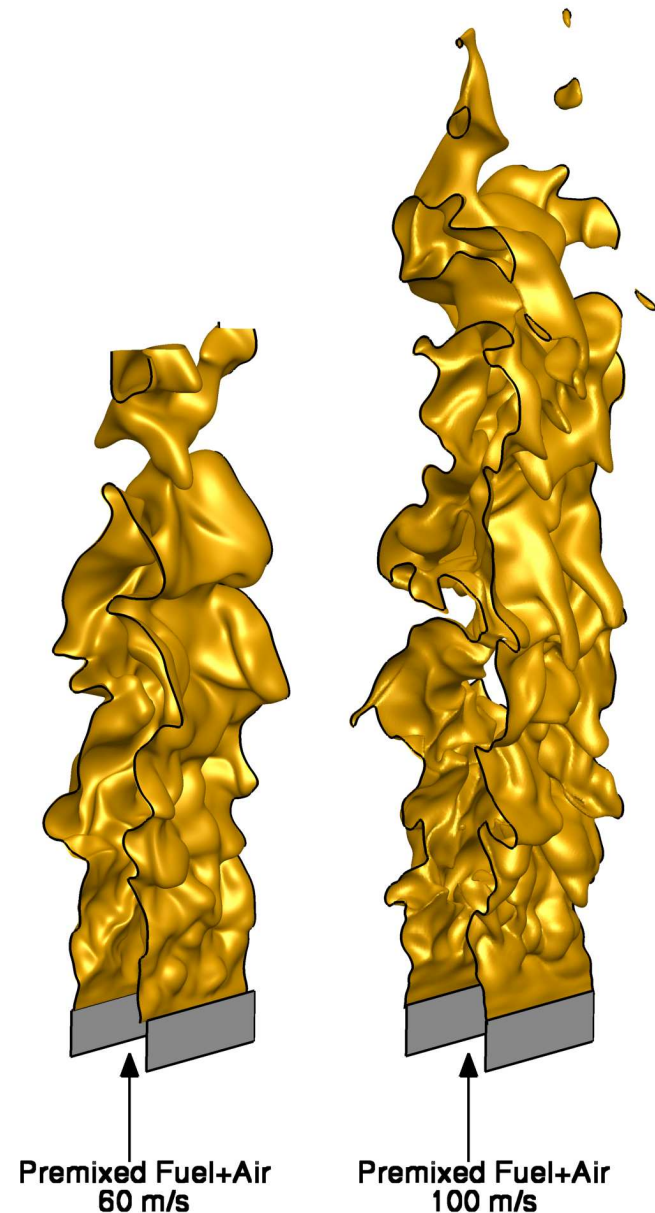


Flame speed (S_L)	1.8 m/s
Flame thickness based on maximum temperature gradient (δ_L)	0.3 mm
Nominal flame thickness (v/S_L)	.05 mm
FWHM of heat-release layer (δ_H)	0.15 mm

	Case 1	Case 2
Jet velocity	60 m/s	100 m/s
Co-flow velocity	15 m/s	25 m/s
Turbulence intensity at inflow (u')	12 m/s	25 m/s
Jet Reynolds no. (Re_{jet})	840	1400
Turbulence Reynolds no. (Re_t)	20	35
Karlovitz Number (δ_L/l_k) ²	100	100
u'/S_L	3	6
l_t/δ_L	0.7	1
Number of Grid points	52M	88M

Simulation Results

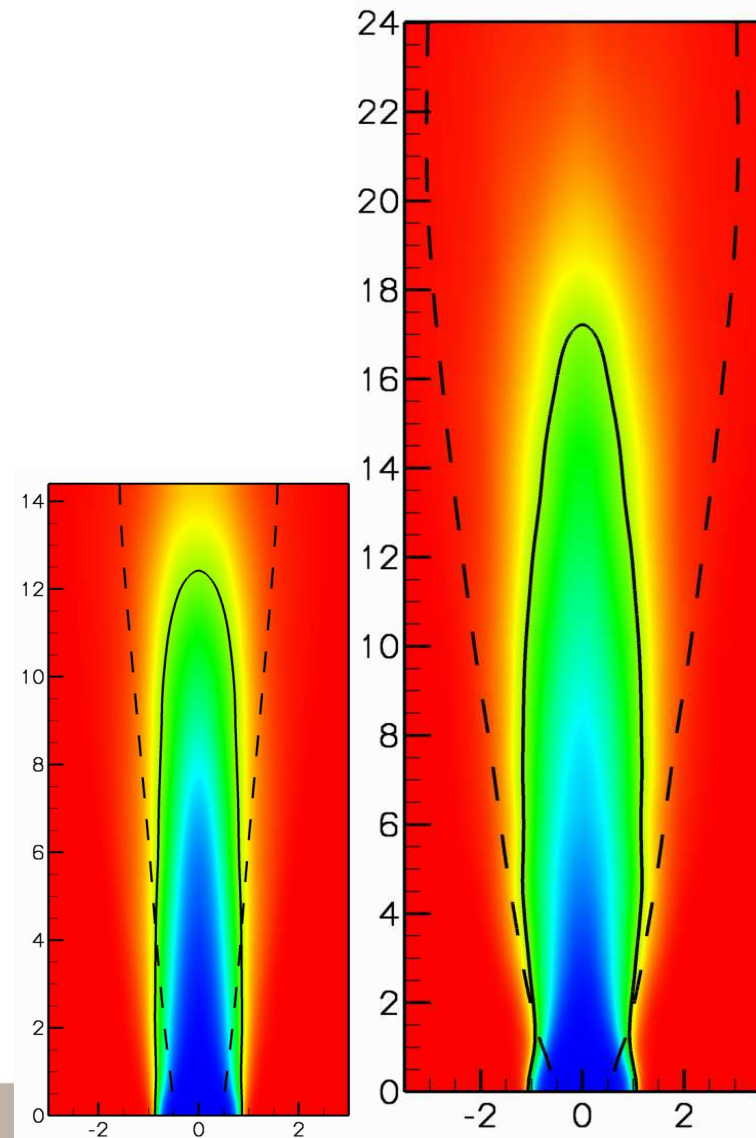
- Significant downstream development of jet
- Mean shear leads to large scale roll-up
- Pinch-off at the tip
- Flame surface is convex towards products
 - Opposite of Huygens propagation
 - Flow straining is more important than self-propagation.
- Results presented at selected stream-wise locations



Mean Flame Brush



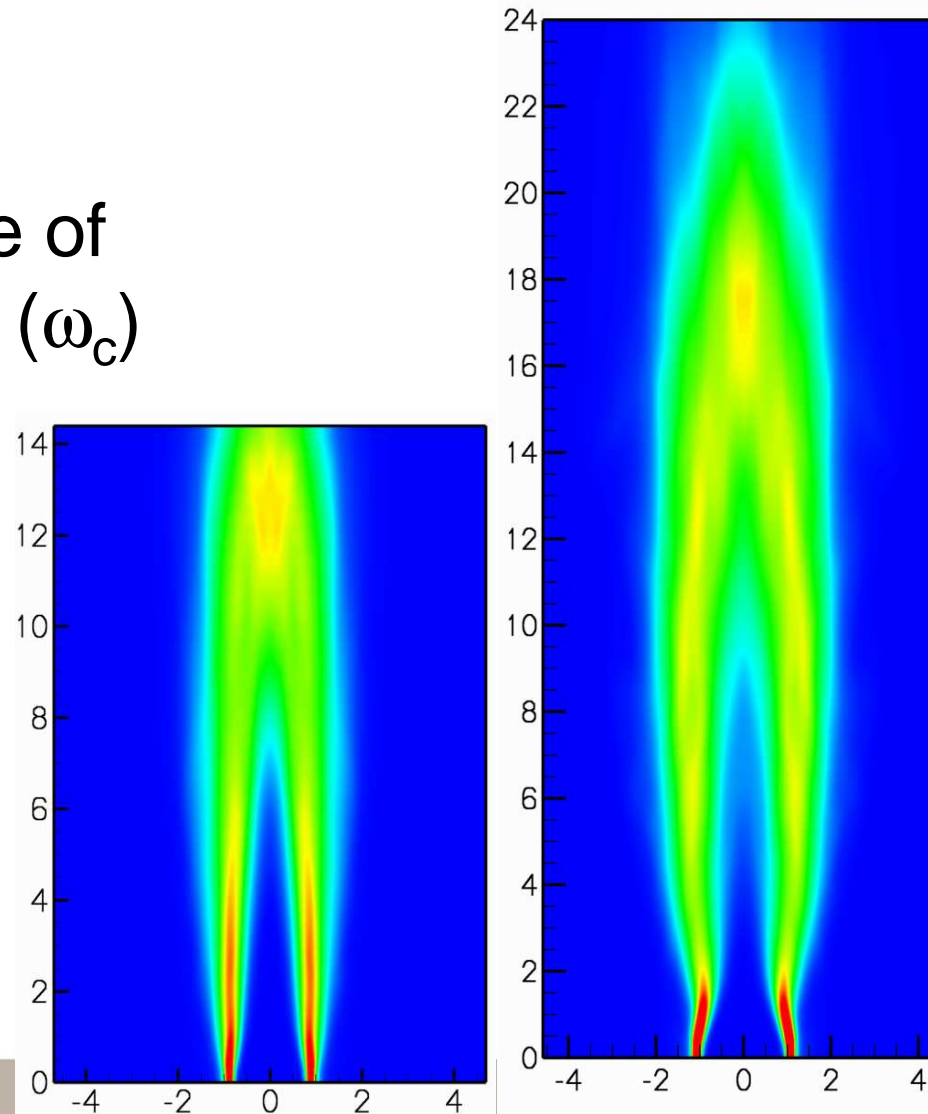
- Progress variable (c) defined based on O_2 mass fraction
- Mean flame properties obtained through averaging in the periodic direction and time.
- Figure shows mean flame brush
 - Color contours indicate the mean progress variable (c) from 0 (blue) to 1 (red).
 - Solid line shows the location of $c=0.65$. (Max. heat release rate).
 - Dashed line shows the location of shear layer. (dU/dy is a maximum)



Mean Reaction Rate



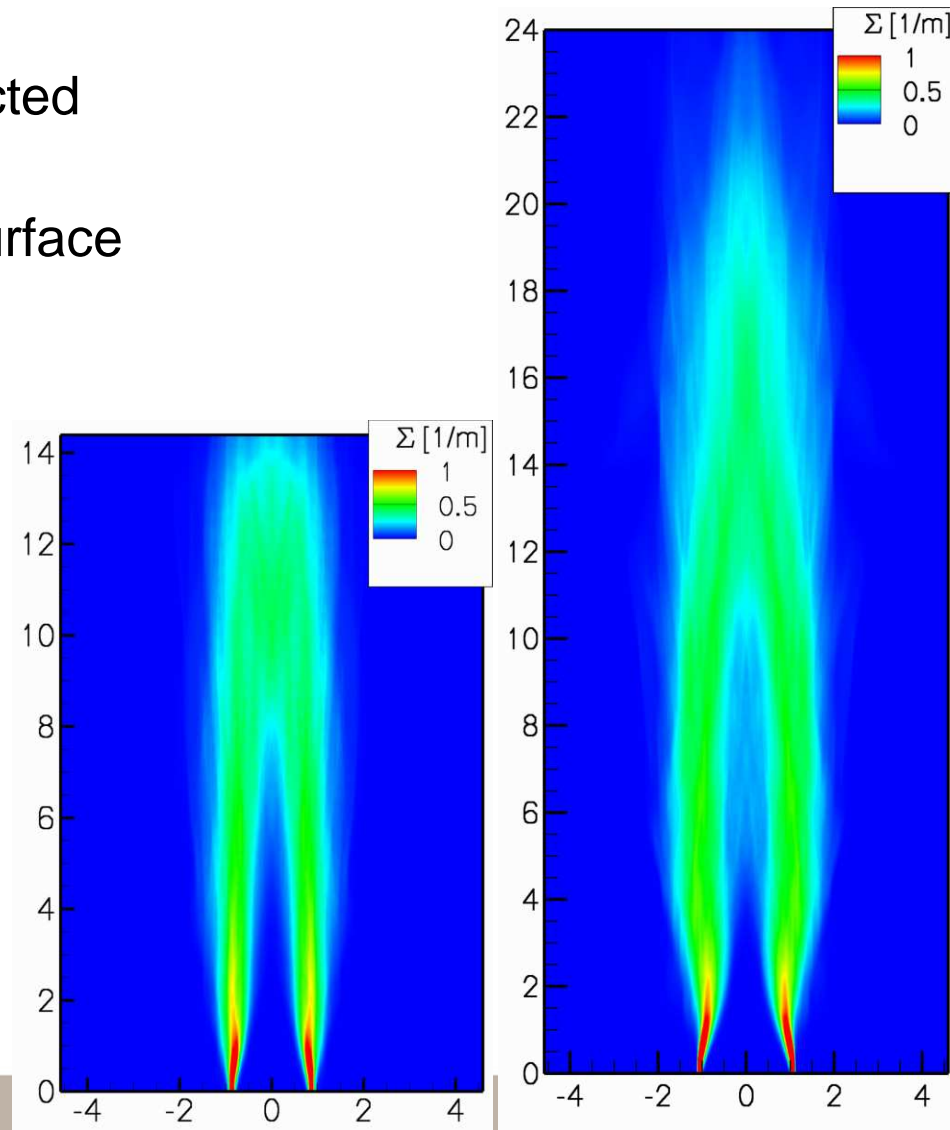
- Mean reaction rate of progress variable. (ω_c)



Flame Surface Density (Σ)



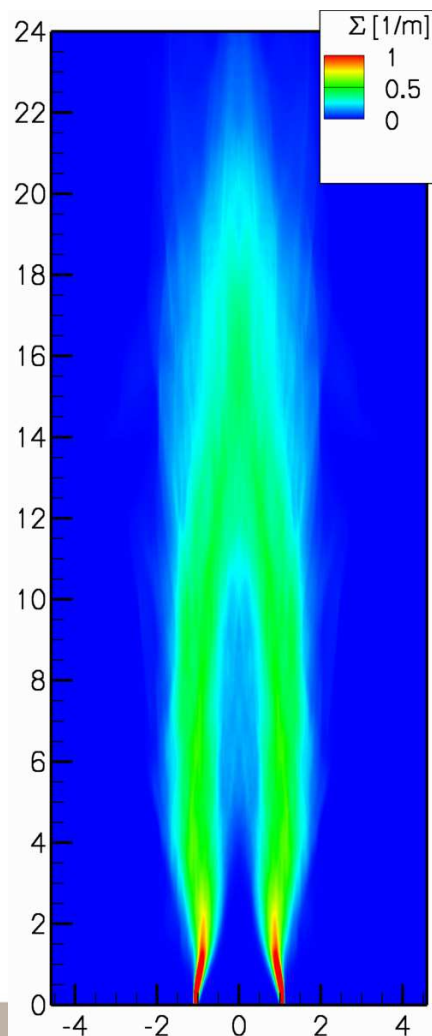
- Isosurface ($c=0.65$) extracted through triangulation.
- Local Σ computed from surface area.



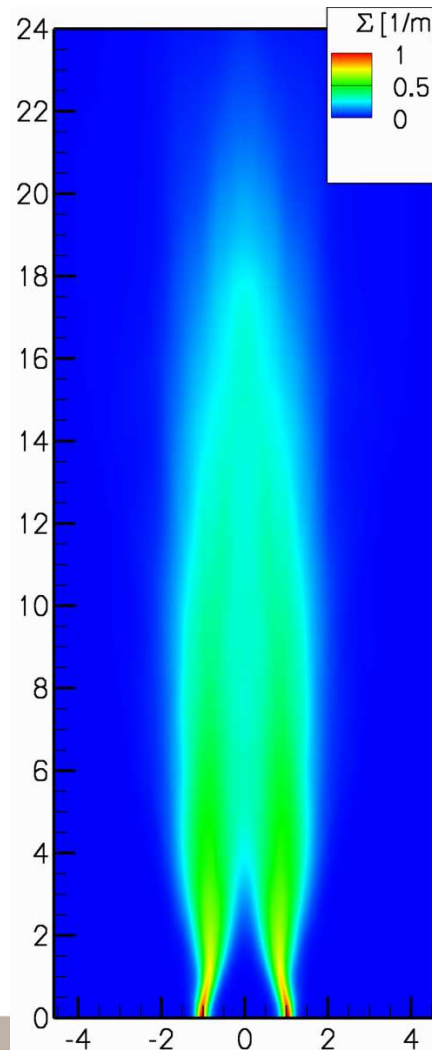
Effect of definition of Σ



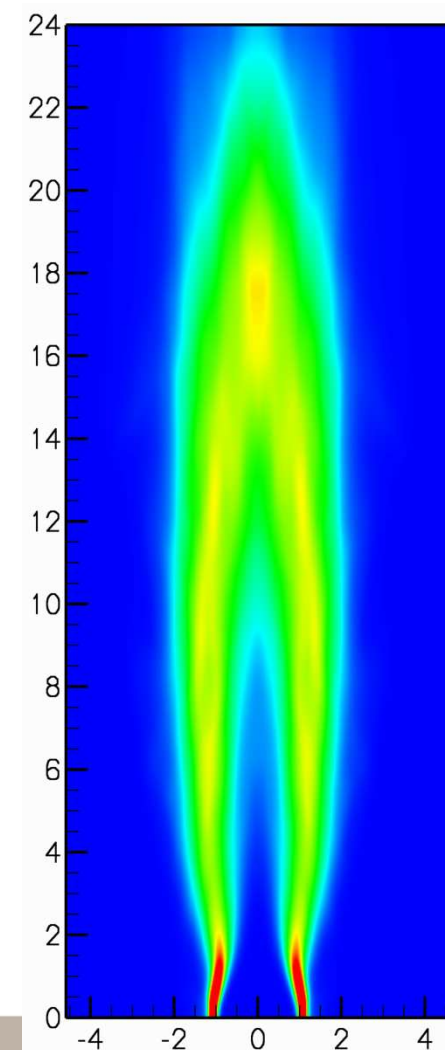
From isosurface



$\Sigma = \langle |\nabla c| \rangle$



$\langle \omega_c \rangle$

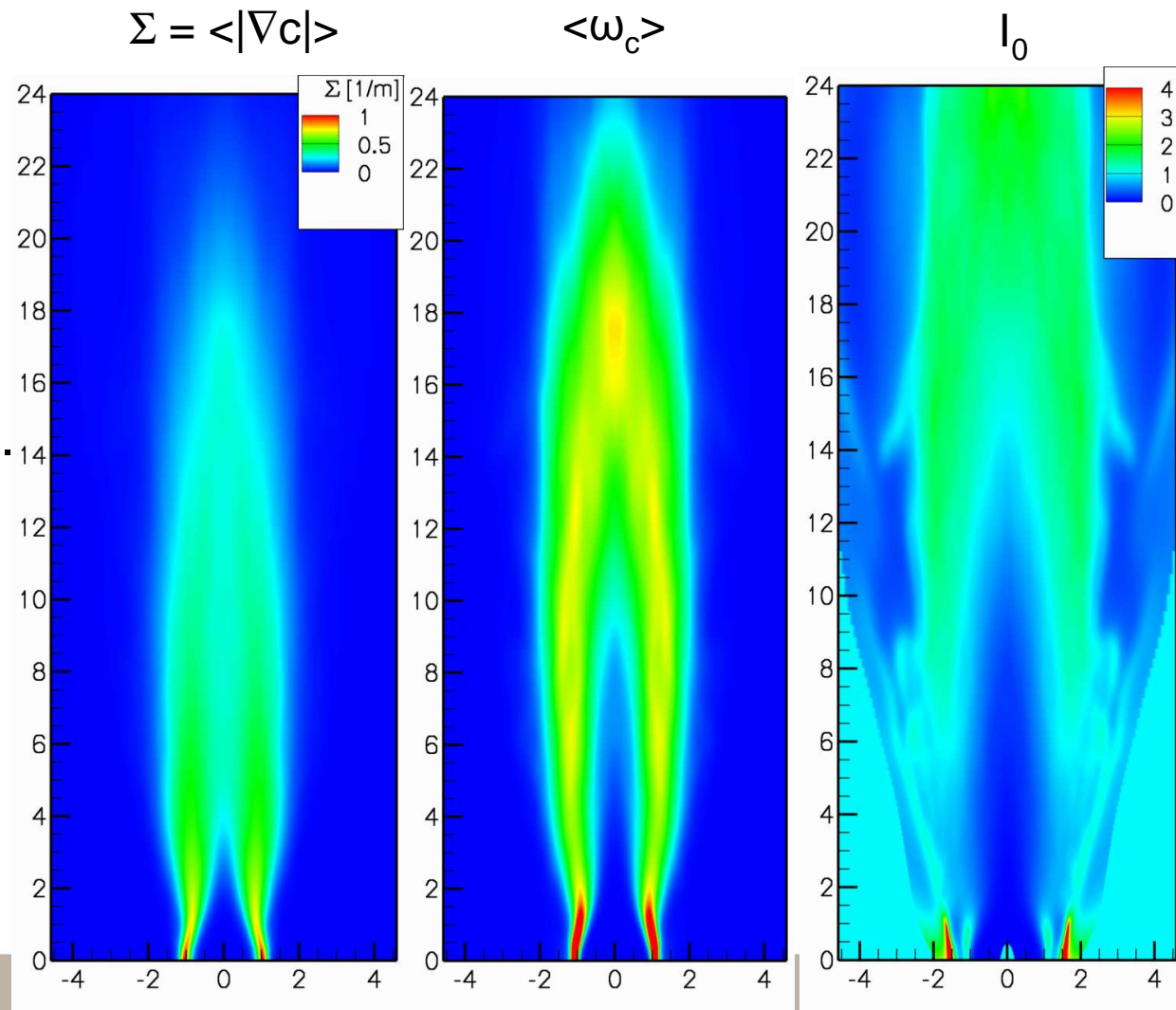


Efficiency Factor (I_0)



$$\dot{\omega} = \rho_0 S_L I_0 \Sigma$$

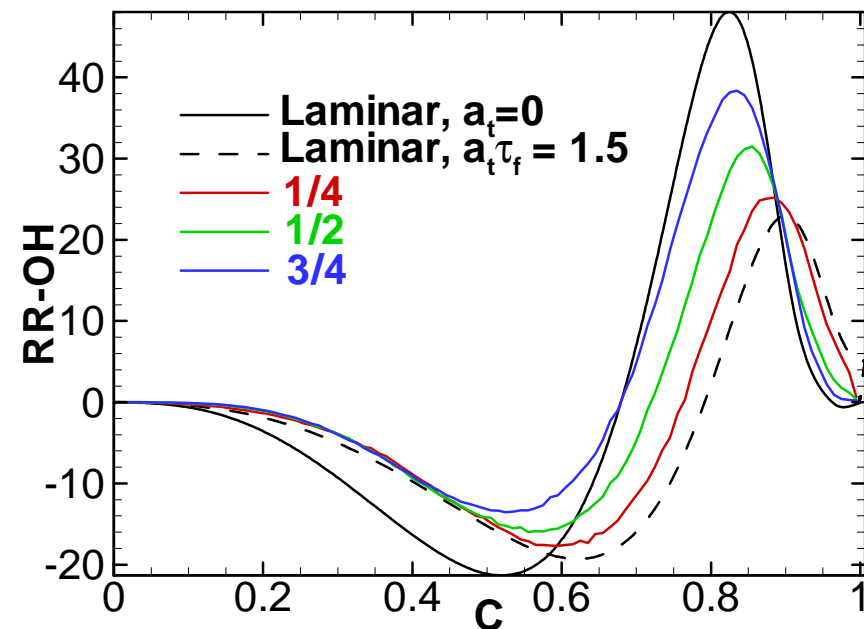
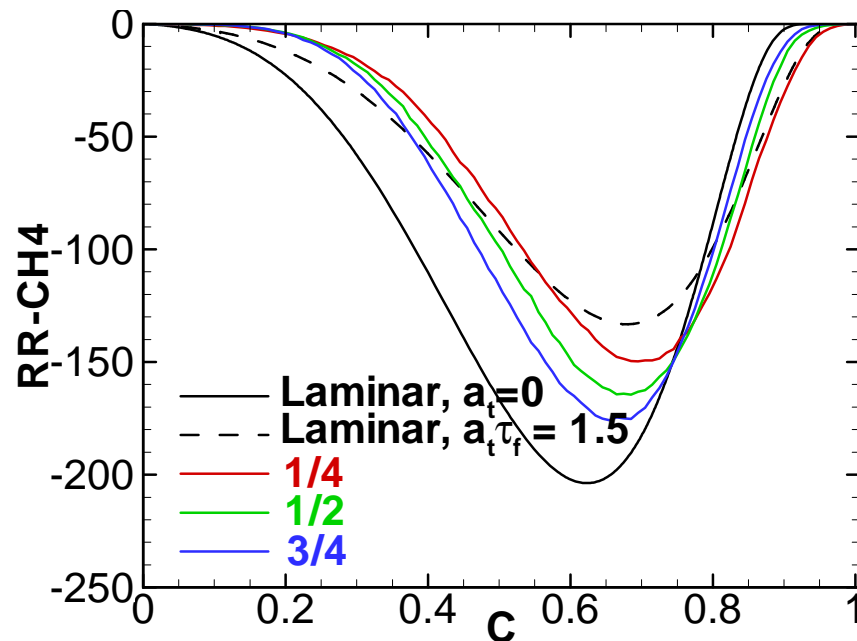
- I_0 represents increase in reaction rate per unit surface area.
- Seems to increase at tip.
- Effect of mean stretch?



Effect on Reaction Zone



- Did turbulence affect the reaction layer?
- Conditional average reaction rates fall between laminar solutions.
- Lack of significant influence on reaction zone
 - Dissipation of turbulence due to heat release?

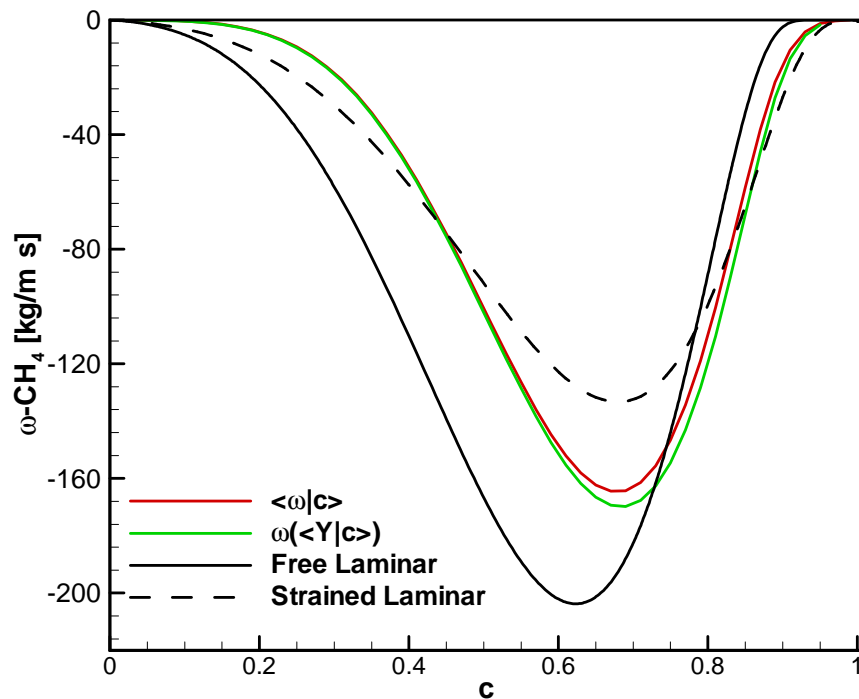


Maybe CMC will work?

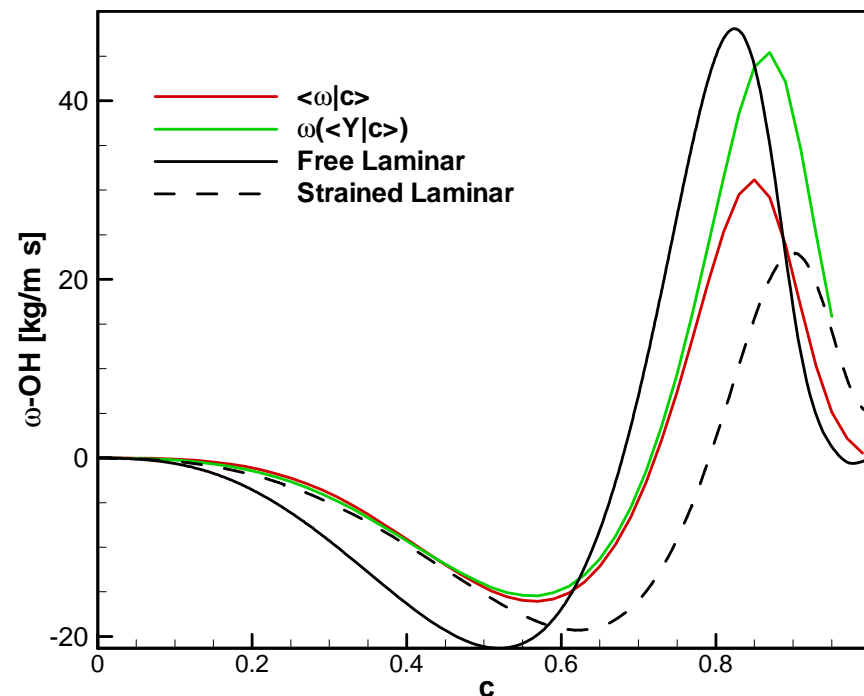


Basic CMC a priori test: $\langle \omega(Y, T) | \eta \rangle \approx \omega(\langle Y | \eta \rangle, \langle T | \eta \rangle)$

CH₄



OH



- Progress variable based on O₂
- Great for major species
- Some deviation on burned gas side for OH, but pretty good.

Direct Numerical Simulation of Flame-Wall Interaction

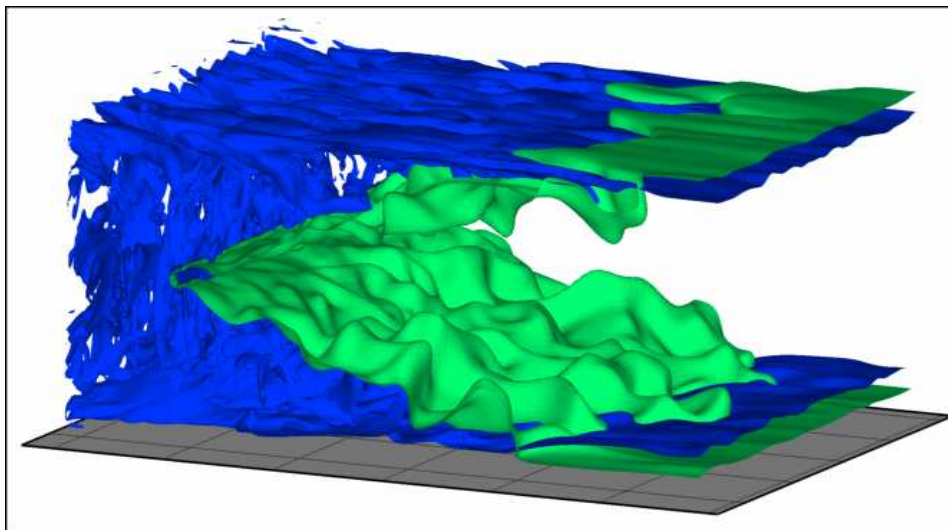


FWI-processes not fully understood as of yet and their role is important in:

- Wall Heat Flux
- Unburned fuel / pollutant emissions

DNS configuration:

- Anchored H_2 -air flame at $\phi=1.5$
- Reactants preheating at $T=750K$
- Turbulent Poiseuille Flow at $Re_t=180$
- Damkohler number ~ 0.26
- Grid $630 \times 200 \times 280 \sim 32$ Mill. Points
- Computational Domain $7h \times 2h \times 3h$
- $\Delta x^+=2$, $\Delta y^+=0.5-3.4$, $\Delta z^+=2$
- Flame anchored at $y^+=180$
- Temporal length of 2 transit-times



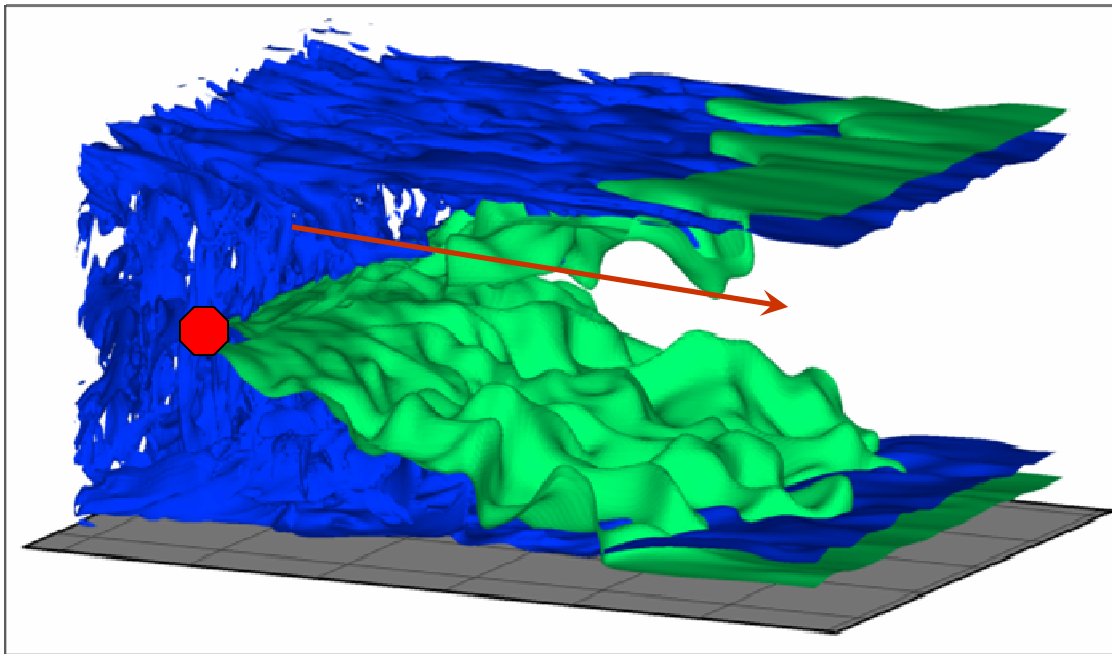
Main conclusions from visual inspection and spectral analysis of the solution:

- Wall Heat Flux Spatial and Temporal Patterns Caused by Near-Wall Turbulent Structures
- Exothermic Radical Recombination Reactions at the Wall Responsible for the Large Wall Heat Fluxes

Improved Boundary Condition Treatment



- ❑ Turbulence Feeding Mechanism:
 - Feed clean evolved turbulence from a non-reacting simulation
 - High turbulence intensity relative to mean convective velocity
- ❑ Entrainment and flame impingement on outflow boundary
- ❑ Nonreacting and reactive wall boundary treatments
 - Coupling of surface kinetics with gas-phase kinetics



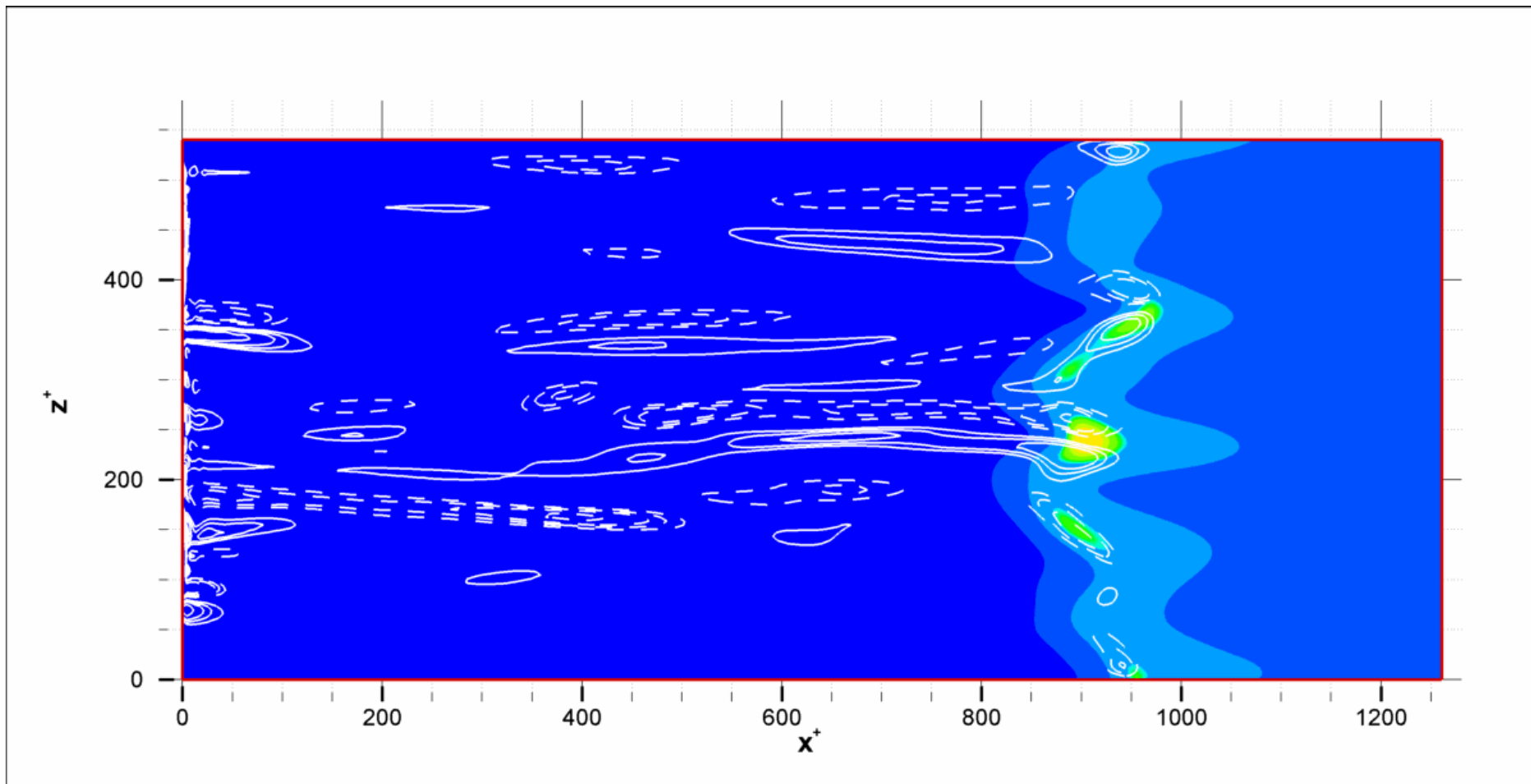
Premixed H₂/air
Flame Wall
Interaction (V-
flame in a
Channel Flow)

*Gruber et al.
2006*

Instantaneous Wall Heat Flux



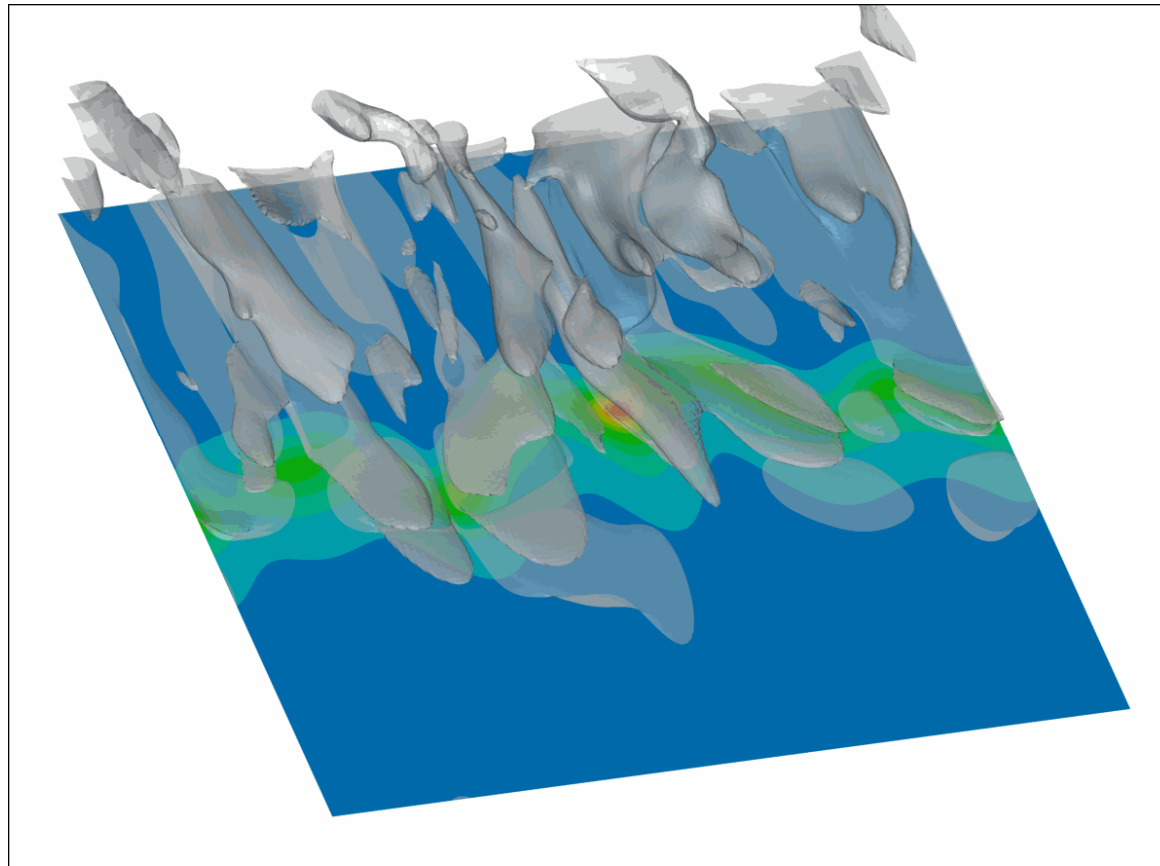
Color scale: wall heat flux. Isolines: Wall normal vorticity at $y^+=5$



Instantaneous Wall Heat Flux



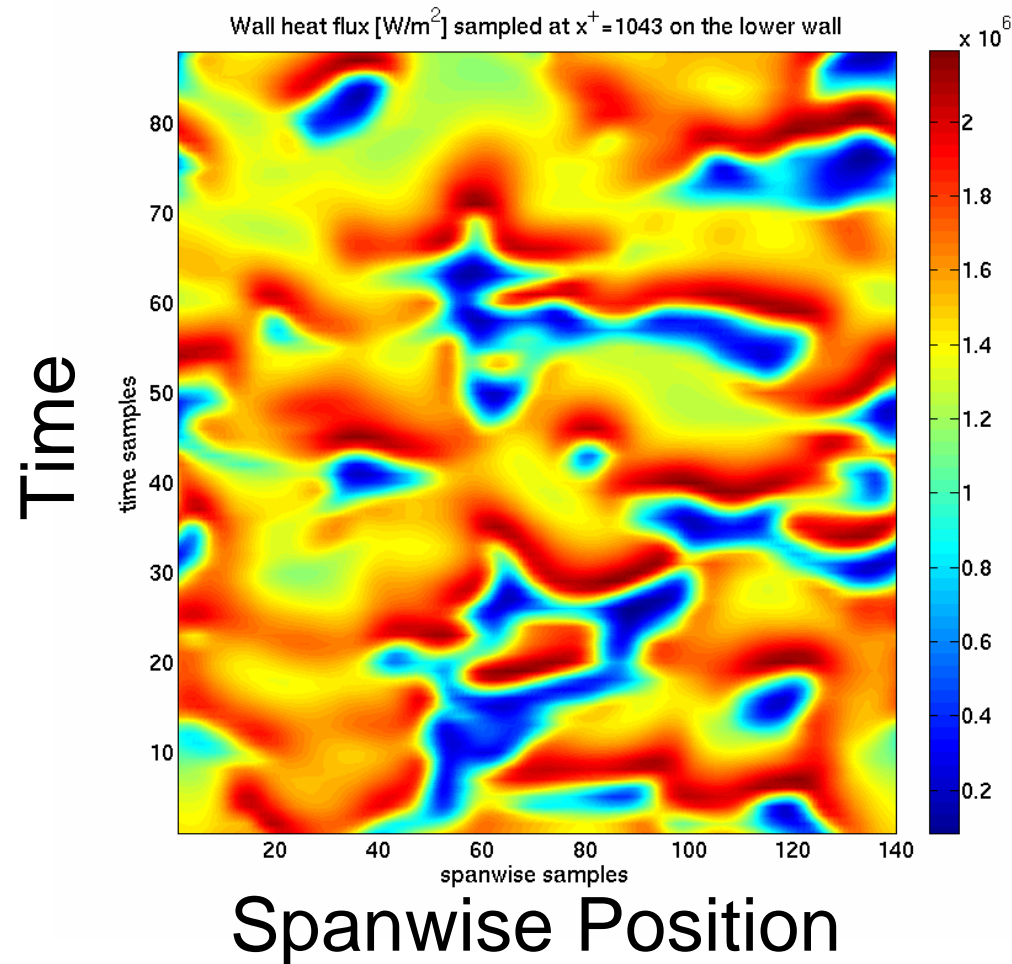
Color scale: Wall heat flux. Isosurfaces: Streamwise vorticity.



Instantaneous Wall Heat Flux Raw Data



- Data reduction:
Sample only at maximum average wall heat flux location



Temporal and Spatial Spectra of the Instantaneous Wall Heat Flux

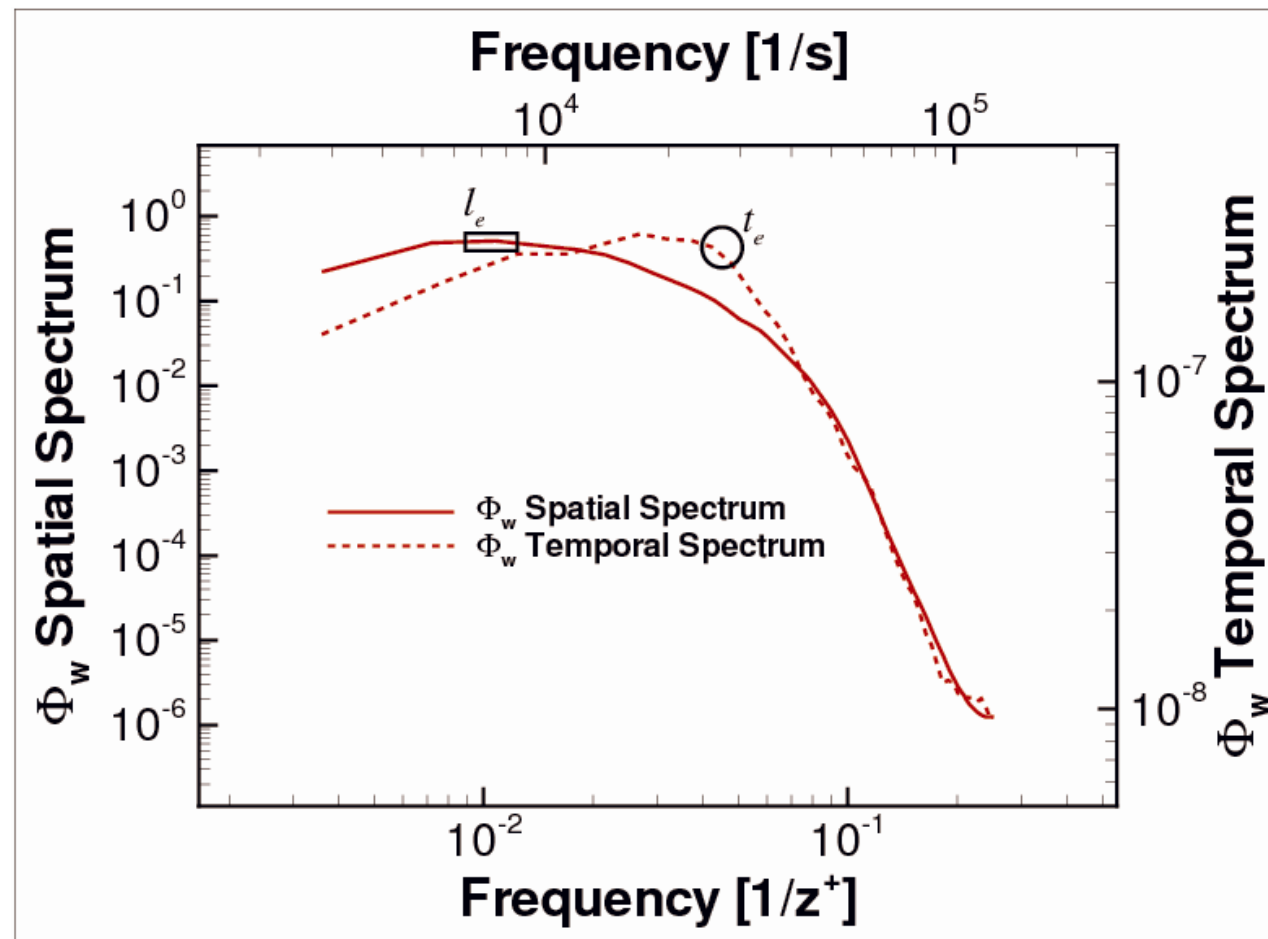


$1/l_e \sim 100$ viscous lengths,
relevant range between
 $1/50$ and $1/200$

$1/t_e \sim h/U_c$, relevant range
between $t^+ \sim 10$ and $t^+ \sim 26$

$t^+ \sim 16 \rightarrow$ structure
“turnover time”

$t^+ \sim 26 \rightarrow$ structure
“passage time”:
 $(300 x^+) / (11 u^+) \sim 26 t^+$





Thanks!

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Flame-Wall work: Andrea Gruber

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